# Localization in two- and three-dimensional systems away from the band center

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Extensive numerical results using finite-size-scaling methods for two-dimensional (2D) and three-dimensional (3D) disordered systems are presented for eigenenergies $E$ different from zero. Single-parameter scaling law is satisfied for all of our results in both 2D and 3D systems. In 2D we find only localized states, however, the localization length does not have its maximum at the band center. In 3D, the dependence of the mobility edge on the strength of the diagonal order is obtained. These results are found to be in satisfactory agreement with the predictions of the coherent-potential approximation and the potential-well analogy.

## I. INTRODUCTION

In the last ten years a number of analytical[1] and numerical techniques[1,2] have been developed to study the problem of Anderson localization in disordered systems. In spite of the extensive studies our ability to obtain explicit quantitative results is limited. Recently an analogy of the localization problem with that of a bound state in a potential well was developed[3] through a diagrammatic analysis of the conductivity[4] in the disordered systems. The analogy with the potential well permits explicit calculations of the localization lengths, conductivities, mobility edges,[3] etc., from quantities that can be obtained from mean-field theories, such as, the coherent-potential approximation[5] (CPA). However, in order to check results of the approximate scheme outlined above [based on the CPA and the potential-well analogy (PWA)], we need independent methods of obtaining the same quantities. Up to now, the most reliable approach is probably the strip or wire method.[2,6-8] In this method, one considers coupled one-dimensional systems (1D). Each 1D system is described by a tight-binding Hamiltonian of the form

$$H=\sum_n |n\rangle\epsilon_n\langle n| + V\sum_{nm}{}' |n\rangle\langle m| \ , \tag{1}$$

where $\epsilon_n$ are independent random variables with a common probability distribution. In our explicit results, we assume that the probability distribution is rectangular of total width $W$. The corresponding sites of the nearest-neighbors 1D system are coupled together by an interchain matrix element. As the number of coupled chains approaches infinity, we recover either the two-dimensional (2D) system when the chains are placed on a plane with two nearest neighbors each or the three-dimensional (3D) system when they are placed to form a cylinder of square cross section.

In this paper we examine the nature of eigenstates in both 2D and 3D disordered systems with diagonal disorder by using an iterative method applied to very long strips of finite width $M$ combined with finite-size scaling methods. In particular, we are interested in testing the single parameter scaling theory[9] for eigenenergies $E$ different from zero. (Most of the numerical work[2,6-8] to date has been done only for $E=0$.) We are interested also in checking how accurate the results obtained by an approximate scheme based on the coherent-potential approximation and the potential-well analogy are. Our numerical results for 2D show, as is now well accepted, that all eigenstates are exponentially localized. However, we find that the localization length $\lambda$ as a function of energy for constant disorder has a maximum not at $E=0$ as one might expect but at $E\neq 0$. The exact value of energy at which $\lambda$ has its maximum value depends on the amount of disorder. For 3D, we numerically calculate for the first time the mobility edge trajectory in the energy-disorder plane for the tight-binding model. This trajectory is in good agreement with our previous prediction (see Fig. 5 of Ref. 3) based on the PWA. Our numerical calculations of localizations length $\lambda$ and correlation length $\xi$ are in qualitative agreement with the results obtained from the PWA. The quantity $\xi$, which characterizes the largest extent of the amplitude fluctuation of an extended eigenfunction, can be defined from the relation $\lambda_M=M^2/c\xi$, where $\lambda_M$ is the largest localization length in a wire of cross-section $M^2$, and $c\approx 4.8$ is a constant determined by the requirement that $\xi$ diverges in the same way as $\lambda$ near the critical point. Finally, for the 3D case, we find that finite-size scaling is obeyed for all $E$'s and $W$'s in agree-

 

ment with the scaling theory ideas of Abrahams *et al.*[9]

For the 2D (3D) case, our system consists of $M(M^2)$ regularly placed chains, of length $N$, each having two (four) nearest neighbors. Then, one determines through a rather sophisticated numerical technique[6–8] the largest localization length $\lambda_M$ for 2D (3D) systems with $M(M^2)$ coupled chains, as $N\to\infty$, respectively. The largest $M$ for which reliable numerical determination of $\lambda_M$ has been carried out is $M=32$ for 2D and $M=8$ for 3D. One finds two distinct behaviors of the function $\lambda_M$ versus $M$. In the first case, which corresponds to a localized state, the second derivate $d^2\lambda_M/dM^2$ is negative and $\lambda_M$ approaches a finite value $\lambda$ as $M\to\infty$, where $\lambda$ is the localization length of the resulting 2D (3D) disordered system. In the second case, which corresponds to an extended state, $d^2\lambda_M/dM^2$ is positive and $\lambda_M\to\infty$ as $M\to\infty$.

## II. TWO-DIMENSIONAL RESULTS

MacKinnon and Kramer[7] have studied numerically the quantity $\lambda_M$ for the center of the band; $E=0$. They found that the function $\lambda_M$ versus $M$ obeys a simple scaling relation of the form

$$\frac{\lambda_M}{M}=f_d\left[\frac{\lambda}{M}\right], \tag{2}$$

where $d$ is the dimensionality, and $f_d(x)$ is a universal function of its argument. They also determined[7] numerically the form of the function $f_d(x)$ and the dependence of $\lambda$ on the disoder $W$. They found that $f_d(x)$ is an increasing function of $x$ with

$$f_d(x)\to cx \quad \text{as } x\to 0\,, \tag{3}$$

where obviously $c=1$.

We calculated $\lambda_M(E,W)$ for $d=2$ and $W=5$ for energies in the range $1<E<6$ and $M=2$, 3, 6, 8, 16, and 32. In agreement with the $E=0$ case, examined by MacKinnon and Kramer,[7] we find that all of our results for $\lambda_M$ with $E\neq 0$ tend to follow the one parameter scaling assumption given by Eq. (2). In Fig. 1 we plot the scaling function $f_2(x)$ obtained by MacKinnon and Kramer for $E=0$ together with our points, which correspond to various energies, disorders, and widths $M$. Although our points are clustered around the MacKinnon-Kramer curve, there is considerable dispersion due to numerical errors, which are appreciable because we are dealing with rather large $\lambda$ or $\lambda_M$ in most of the cases. As a result of these uncertainties, we estimate that our numerical results for $\lambda$ plotted in Fig. 2(a) are no more accurate than 10–20% for large localization lengths. Near the tails where $\lambda$ is small, the relative error is much lower, i.e., about 2%. This uncertainty could be reduced somehow at the expense of increasing substantially the computer time. (An error of about 2% in $\lambda_M$ requires the length $N$ to be $10^4$ times the localization length $\lambda_M$.)

For $E=0$ we found $\lambda\approx 110$ which agrees within numerical uncertainties with the values 110 and 97.58 obtained by MacKinnon and Kramer in Ref. 7. Note that $\lambda$ has a maximum at an energy different than zero. In particular, for the case of $W=5$, $\lambda$ has a maximum at $E=2.0$ and then drops rapidly as the energy $E$ increases. One might have expected that the states at $E=0$ should be less localized than the states at $E\neq 0$. We believe that the local minimum of the localization length $\lambda$ at $E=0$ reflects the existence of Bloch states with zero group velocity at $E=0$ for the ordered square lattice. The vanishing of the group velocity at $E=0$ is also responsible for the

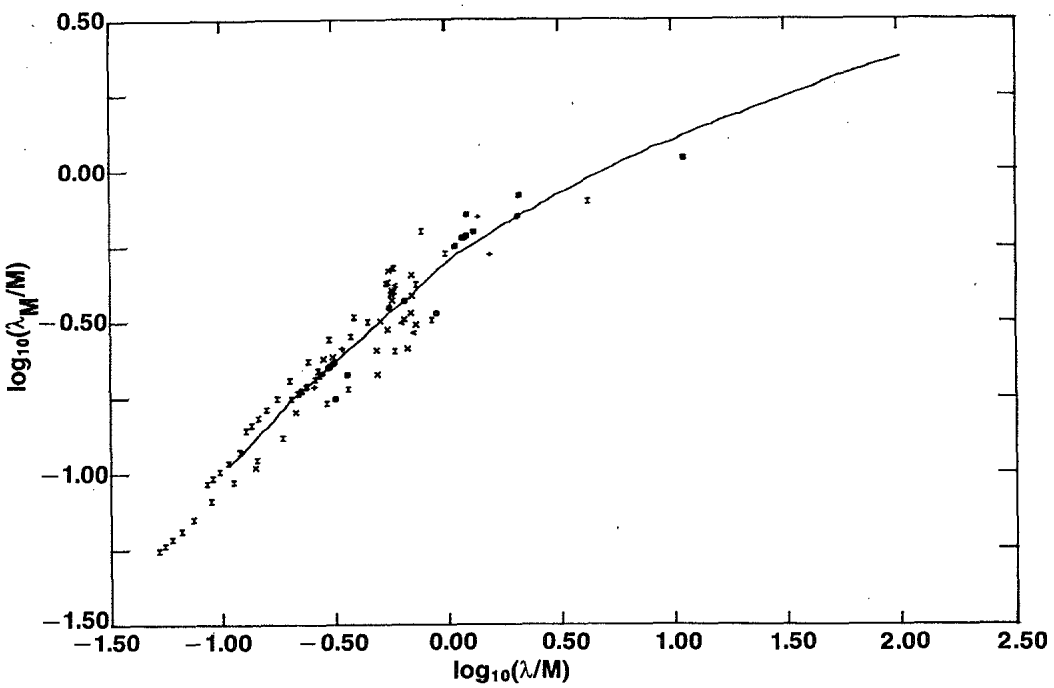


FIG. 1. Renormalized localization length $\lambda_M/M$ vs $\lambda/M$ for various values of disorder $W/V$ and various energies $E/V$ for a square lattice. Solid line represents an average over the data points. There is only one branch in the universal curve, so all states are exponential localized.

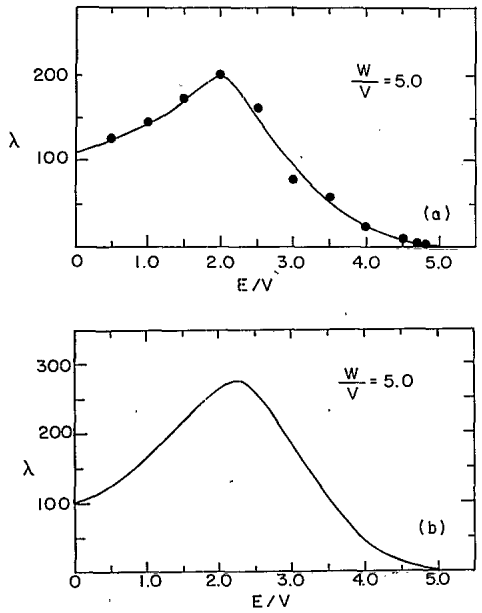


FIG. 2. Localization length $\lambda$ (in units of lattice spacing) versus energy $E/V$ for a square lattice with disorder $W/V=5.0$. (a) gives the numerical results while (b) gives the results from the PWA with the CPA.

appearance of a Van Hove singularity in the density of states at $E=0$ for the ordered lattice. Thus, the reduction of the localization length at the neighborhood of $E=0$ can be attributed to the idea that it is easier to localize a state with zero group velocity. This idea is supported also by our previous calculations in simple-cubic lattices,[3] where a local minimum appears both in the mean free path and the conductivity near the Van Hove singularity for weak disorder. We have also calculated the localization length $\lambda$ by the PWA and the CPA. This is shown in Fig. 2(b). To obtain these results, we have used the simple expression for $\lambda$ derived previously[3] by the PWA,

$$\lambda=2.72l\exp(lS/4)=2.72l\exp(\pi^2\hbar\sigma_0/e^2)\ , \tag{4}$$

where $l$ is the mean free path, $S$ is the area of the Fermi surface, and $\sigma_0$ is the conductivity, all calculated within the CPA. It is worthwhile to point out that Eq. (4), as opposed to the PWA, is valid for low disorder and that other approaches, such as, the scaling method or the summation of maximally crossed diagrams, produce the same exponential factor as in Eq. (4); however, the preexponential factor is less certain. There are even suggestions that it is not proportional to the mean free path $l$. In our previous work, we have concluded that the prefactor $2.72l$ fits best the numerical results of MacKinnon and Kramer[7] for $E=0$. Thus, it is interesting to see whether or not the same formula [i.e., Eq. (4)] could fit results for other energies (and not so large a disorder). Comparison of Figs. 2(a) and 2(b) shows a rather reasonable agreement, although Eq. (4) produces higher values of $\lambda$ near the maximum. However, the numerical results are less certain near the maximum of $\lambda$. Thus, we can conclude that Eq. (4) gives a reasonable estimate of $\lambda$. This reinforces our opinion that the PWA is very useful in obtaining quantitative results for various quantities of interest in disordered systems. From Eq. (4) it is clear that the maximum of $\lambda$ is essentially controlled by the maximum of $\sigma_0$. In the present case, $\sigma_0(E)$ has a local minimum at $E=0$ (for $W$ not so large) due to the Van Hove singularity and approaches zero linearly at the perturbed band edge. In between it must have a maximum, the position of which depends on the disorder. This behavior of $\sigma_0(E)$ fully accounts for the behavior of $\lambda$ versus $E$ as shown in Fig. 2.

In the weak disorder limit ($W\ll 4V$) and for $E$ near the perturbed band "edge" (but inside the band) the CPA can be approximated by its lower-order expansion,

$$\Sigma\approx\frac{W^2}{12}G_0(E-\Sigma)\ , \tag{5}$$

and $G_0(E)$ by

$$G_0\approx\frac{1}{4\pi V}\ln\left[\frac{-E}{32V}\right]\ , \tag{6}$$

where $E=0$ corresponds to the *lower* unperturbed band edge. By combining Eqs. (5) and (6) we find that the band edge is shifted by an amount $E_{\rm CPA}$ given by[10]

$$\begin{aligned}E_{\rm CPA}&\approx\frac{W^2}{24\pi V}\left[\ln\left[\frac{W}{16\sqrt{6\pi}V}\right]-\frac{1}{2}\right]\\&\approx\frac{W^2}{24\pi V}\left[\ln\left[\frac{W}{69.466V}\right]-\frac{1}{2}\right]\ .\end{aligned} \tag{7}$$

The mean free path $l$ (in units of atomic spacing) can be approximated by

$$\begin{aligned}l=&\frac{V^{1/2}}{2\,|E'|^{1/2}+W/(12\pi V)^{1/2}}\\&+24\sqrt{2}\,\frac{V^{3/2}(E'+|E'|)^{1/2}}{W^2}\ ,\end{aligned} \tag{8}$$

where $E'=E-E_{\rm CPA}$. Taking into account that the Fermi line is given by (in units of atomic spacing)

$$S\approx 2\pi(E'/V)^{1/2}\ , \tag{9}$$

we obtain

$$\sigma_0\approx\frac{e^2}{\hbar}\frac{24}{\pi}\frac{VE'}{W^2},\quad E'>0\ . \tag{10}$$

Substituting Eqs. (8) and (10) in Eq. (4) we obtain an approximate analytic expression for $\lambda$,

$$\lambda=2.72l\exp\left[24\pi\frac{VE'}{W^2}\right]\ . \tag{11}$$

Equation (11) is in good agreement with the exact CPA result for $E$ near and inside the band edge even for $W=5V$.

## III. THREE-DIMENSIONAL RESULTS

For the 3D tight-binding model with diagonal disorder, we calculated $\lambda_M$ for several values of the eigenenergy $E$ and strength of the diagonal disorder $W$ for $M=2$–$7$. From our numerical data, we found that indeed the function $\lambda_M$ versus $M$ obeys the simple scaling relation in Eq.

(2) for localized states, while the extended states follow a different branch[10] of the universal curve shown in Fig. 3. We see from the upper branch of $f_3(x)$ (corresponding to extended states) that $\lambda_M/M$ increases with increasing $M$ and that $\lambda_M \to M^2/c\xi$ as $M \to \infty$, where $\xi$ is the correlation length, $c \approx 4.8$ (and $x = \xi/M$). For all of the cases we examined the scaling function $f_3(x)$ for 3D has the following form as $x \to \infty$:

$$f_3(x) \to 0.6 \quad \text{as } x \to \infty \ . \tag{12}$$

In the opposite limit $x \to 0$, $f_3(x) \sim 1/x$ for extended states [while for localized states $f_3(x) \sim x$]. Using the strip or wire method, we have calculated for the first time the dependence of the mobility edge on the disorder $W$, Fig. 4, for the 3D simple-cubic tight-binding model with diagonal disorder. The points are the numerical results while the solid line is the predictions[3] of the PWA combined with the CPA. The thin solid line gives the CPA band edge. The agreement between the numerical work (which has an error of about 10%) and the PWA is very impressive for the whole trajectory of the mobility edge. The question of the determination of the mobility edge trajectory has a long history. Initially, starting with Anderson's basic paper,[11] the emphasis was to determine a single point of the trajectory, namely, the one corresponding to the center of the band ($E=0$, $W_c$). Estimated values for $W_c/V$ for a simple-cubic lattice were covering a wide range: 62 (Ref. 11), 32.6 (Ref. 12), 20–40 (Ref. 13), 22 (Ref. 14), $\leq 24$ (Ref. 15), 14.5 (Ref. 16). The numerical work of Weaire and Srivastava[17] gave $W_c/V \approx 15$, while the most recent work of MacKinnon and Kramer produced a value of $W_c/V = 16.5 \pm 0.5$. A result for the whole trajectory was first obtained by Ziman,[12] followed

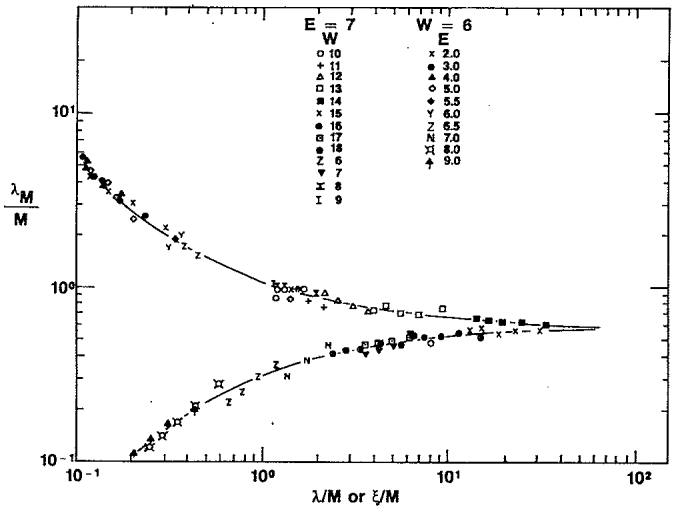


FIG. 3. Renormalized localization length $\lambda_M/M$ vs $\lambda/M$ or $\xi/M$ for various values of disorder $W/V$ and various energies $E/V$ for a simple-cubic lattice. Solid lines represent an average over the data points. There are branches in the universal curve, the upper one corresponding to extended states and $\xi/M$ and the lower one to localized states and $\lambda/M$. Thus, mobility edges exist.

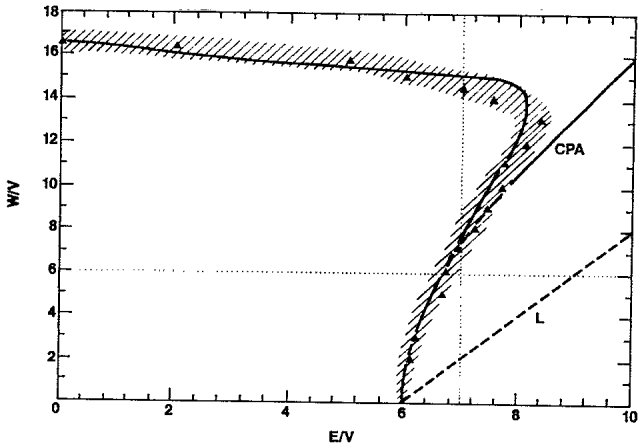


FIG. 4. Dependence of the mobility edge on the strength of the diagonal disorder $W$ for the simple-cubic lattice. Solid triangles are the numerical results. Thick solid line is the prediction of the PWA with the CPA. The CPA band-edge trajectory is also indicated (thin solid line) together with the true (Lifshitz) band-edge trajectory (thin dashed line). The dotted straight lines indicate the independent variables for Fig. 5.

by Economou and Cohen,[14] and by Licciardello and Economou;[16] the last two are based on the so-called $L(E)$ method. More recently, Prelovsek[18] calculated the mobility edge trajectory based on an approximate treatment of kinetic equations for electron density fluctuations; he found a value of $W_c/V \approx 10$. Also, Kotov and Sadovskii[19] and Economou *et al.*[3] obtained the mobility edge trajectory based on a self-consistent diagrammatic technique and the PWA, respectively. In these approaches there is an adjustable parameter of the order of unity which in Ref. 3 was chosen to be 0.75 in order to obtain $W_c/V = 16.5$.

The present numerical results clearly show that the $L(E)$ method of Licciardello and Economou[16] and the PWA[3] produce the best results for the mobility edge trajectory. The $L(E)$ method produces a mobility edge trajectory exhibiting a slight minimum at the center of the band (see Fig. 5 of Ref. 3) in disagreement with the numerical data which show a slight maximum at the center of the band; otherwise, the $L(E)$ trajectory follows the numerical points very faithfully. It is worthwhile to recall that no adjustable parameter whatsoever is involved in the $L(E)$ method of Ref. 16. The PWA is producing clearly the best agreement with the data, which within numerical uncertainty follow the PWA mobility edge trajectory (thick solid line in Fig. 4). As it was shown recently,[20] the mobility edge for low disorder follows the CPA band edge (being inside the latter by an amount proportional to $W^4$); meanwhile the CPA band edge increases as $W^2$. This accounts for the original outgoing shape of the mobility edge trajectory. For high disorders (comparable to Anderson's critical value) the density of states is determined more by the probability distribution rather than the lattice structure and hence, is weakly varying over the band (see Fig. 2 of Ref. 3). Other quantities such as the dc conductivity $\sigma_0$ and the mean free path $l$ are also weakly dependent on the energy. The conclusion is that at such high disorders all energies inside the band are al-

most equivalent and as a result, the critical disorder $W_c(E)$ is almost independent of the energy as long as the latter is well within the band in agreement with the numerical data and the results of the PWA or the $L(E)$ method.

In Fig. 5, we plot the localization length $\lambda$ or the correlation length $\xi$ for two representative cases. In Fig. 5(a) $\lambda$ and $\xi$ are plotted as a function of $E$ for $W=6V$. Note that both $\lambda$ and $\xi$ diverge at an energy which gives the position of the mobility edge for that disorder. In Fig. 5(b), $\lambda$ and $\xi$ are plotted as functions of $W$ for $E=7V$. In this particular case, $\lambda$ and $\xi$ diverge at two values of $W$. As $W$ is increased from zero for $E=7V$ in Fig. 4, we enter first a region of no states until we hit the true band-edge trajectory (Lifshitz limit) for $W=2V$ and we enter the extreme tail region where the localization length $\lambda$ is very small and the density of states exponentially small. The density of states remains extremely low until we approach

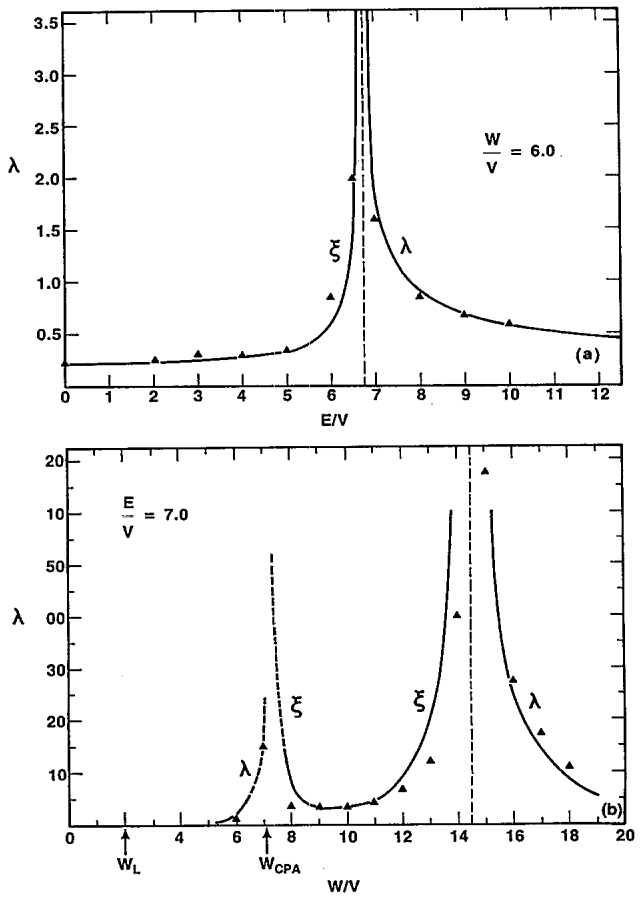


FIG. 5. (a) Localization length $\lambda$ or correlation length $\xi$ as a function of the energy $E/V$ for a simple-cubic lattice with disorder $W/V=6.0$. The solid line is the result of the PWA with the CPA while the triangles are the numerical data. The CPA band edge is just above the critical energy while the true band edge (Lifshitz limit) is at $E/V=9$. (b) Localization length $\lambda$ or correlation length $\xi$ versus the strength of the diagonal disorder $W/V$ for a simple-cubic lattice for energy $E/V=7.0$. The solid line is the PWA result and the triangles are the numerical data. The arrow indicates the position of the CPA band edge. The true band edge (Lifshitz limit) is lower at $W/V=2$. Near the lower critical point results have large uncertainties.

the intersection with the CPA band trajectory $E_{\mathrm{CPA}}$ [denoted by the arrow in Fig. 5(b)]; the $E_{\mathrm{CPA}}$ is a crossover energy where the density of states changes from an exponential to an algebraic dependence. Very close to the $E_{\mathrm{CPA}}$ is the first intersection with the mobility edge trajectory at which the localization length $\lambda$ blows up as shown in Fig. 5(b). For higher disorder, we enter a region of extended states characterized by the correlation length $\xi$; the disorder dependence of the latter is shown in Fig. 5(b). Finally, as we keep increasing the disorder, we cross again for a second time the mobility edge trajectory (see Fig. 4); at this point $\xi$ blows up again. Above this second critical point the states are again localized and are characterized by the localization length $\lambda$, the disorder dependence of which is shown in Fig. 5(b).

The results of the numerical work for $\lambda$ and $\xi$ (represented as triangles in Fig. 5) can be used to check recently obtained formulas[3,21] for $\lambda$ and $\xi$. These formulas were obtained by the PWA and by fitting to numerical results for $E=0$ as to determine the one adjustable parameter in the PWA approach. They are the following:

$$\lambda=\frac{A\phi+B}{1-\phi}l\,, \tag{13}$$

$$\xi=2.72l\left[\frac{1}{\phi}+\frac{6}{\phi^2(\phi-1)}\right], \tag{14}$$

where $\phi=Sl^2/(Sl^2)_c$, $(Sl^2)_c=8.96$, $S$ is the constant energy surface, $l$ is the mean free path, $A=14.12$, and $B=2.20$. Using the CPA to calculate $S$ and $l$ for a given pair of $E$ and $W$ and then substituting into Eqs. (13) and (14), explicit results for $\lambda$ and $\xi$ are obtained. Given the numerical uncertainties of the wire method, and the fact that there is no adjustable parameter in the PWA approach, the agreement in Fig. 5(a) is impressive. In Fig. 5(b) there are some discrepancies between the PWA results and the numerical data. These discrepancies are attributed to the larger numerical uncertainties in the wire method for large $\lambda$ and/or near the critical points. Especially near the lower critical point in Fig. 5(b) the uncertainties in both the PWA and the wire method are larger, because we follow the line $E/V=7$ which crosses the mobility edge trajectory at a very small angle (see Fig. 4) extending thus the critical region from $W\approx 6$ to $W\approx 9$.

## IV. CONCLUSIONS

This paper demonstrates that the potential-well analogy coupled with the CPA is capable of producing results for quantities, such as, $\lambda$ and $\xi$ not only in qualitative but in quantitative agreement with independent numerical data. The discrepancies between the PWA based results and the numerical data are about 10% or less, which is very satisfactory given the uncertainties in the numerical data (which are themselves about 10%) and the previous experience in failing to produce reliable results out of various approximate localization theories.

It must be pointed out that the PWA goes beyond the so-called maximally crossed graphs (MCG) for the conductivity in that it incorporates self-consistency.[3] Because of this self-consistency it can describe not only the weak

disorder case but the strong disorder case as well, where the conductivity depends exponentially on the length of the specimen. This possibility of describing the whole range of disorder is a common feature of all self-consistent approaches originated from the MCG. Because there is no unique way for self-consistency, various self-consistent, post-MCG approaches such as the PWA, the Vollhardt and Wölfle method,[4] and the Kotov and Sadovskii work[19] differ from each other. We think that the PWA is, to date, the most successful self-consistent post-MCG approach. We base this statement on (i) its conceptual simplicity and pedagodic values; (ii) the fact that it reproduces the exact analytical result for the conductivity in the 1D case for all values of the disorder;[22] and (iii) the satisfactory quantitative agreement with independent numerical data on the localization and correlation lengths $\lambda$ and $\xi$, the conductivity $\sigma$, and the mobility edge trajectory; this agreement was demonstrated in our previous work[3,21] for $E=0$ (center of the band) and in the present work for $E\neq 0$ both for two and three dimensions.

Based on the above successes, one can state that the calculation of several important quantities in disordered systems has been reduced to the most elementary problems in quantum mechanics: the gross features, such as, the density of states and the mean free path are obtained from an effective uniform (or periodic) medium (determined from the CPA condition); the more refined aspects due to fluctuations around this effective medium, such as, localization length, correlation length, position of the mobility edge, and conductivity, are obtained by the simplest possible departure from uniformity, i.e., by a simple effective potential well (which is again determined by the CPA).

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